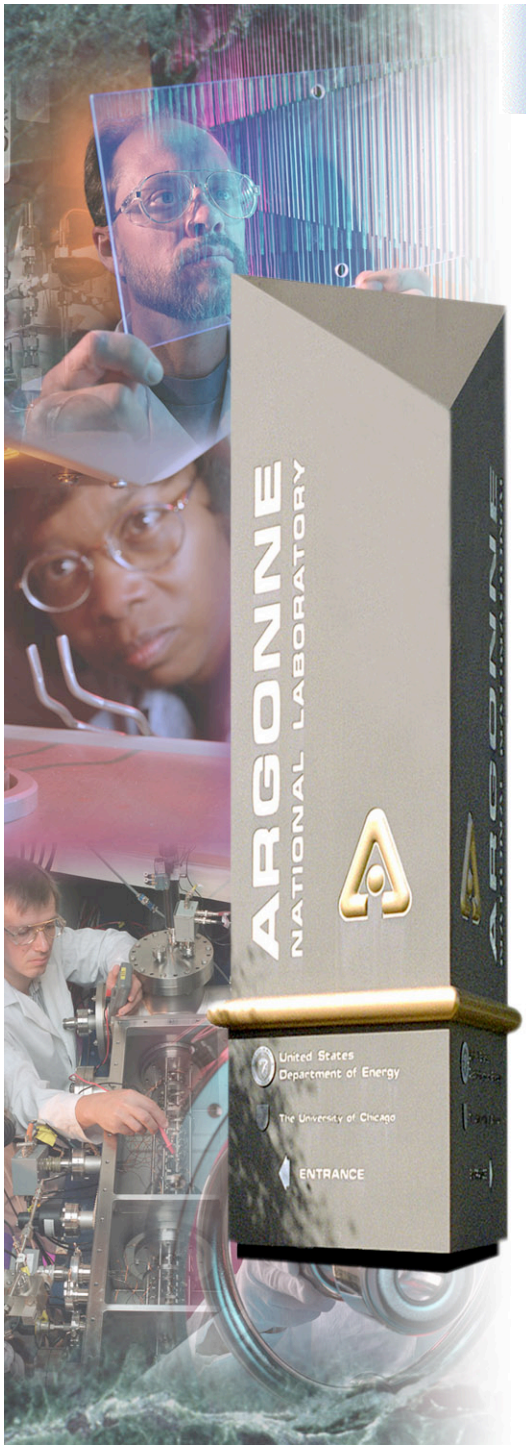


ARGONNE NATIONAL LABORATORY

# *Chemical Reprocessing Plant Simulation*

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Advanced Simulations: A Critical Tool for Future Nuclear Fuel Cycles

Lawrence Livermore National Laboratory
December 14-16, 2006

THE UNIVERSITY OF CHICAGO

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## *Objective*

- Combine chemical, engineering, and operational expertise to develop the capability to design, simulate, and optimize an aqueous nuclear processing facility
- Enable the design of a facility that is chemically, operationally, and economically efficient
- Integrate the process and facility design with systems analysis to examine regulatory, economic, physical, and environmental impacts

# *Approach*

**Current**

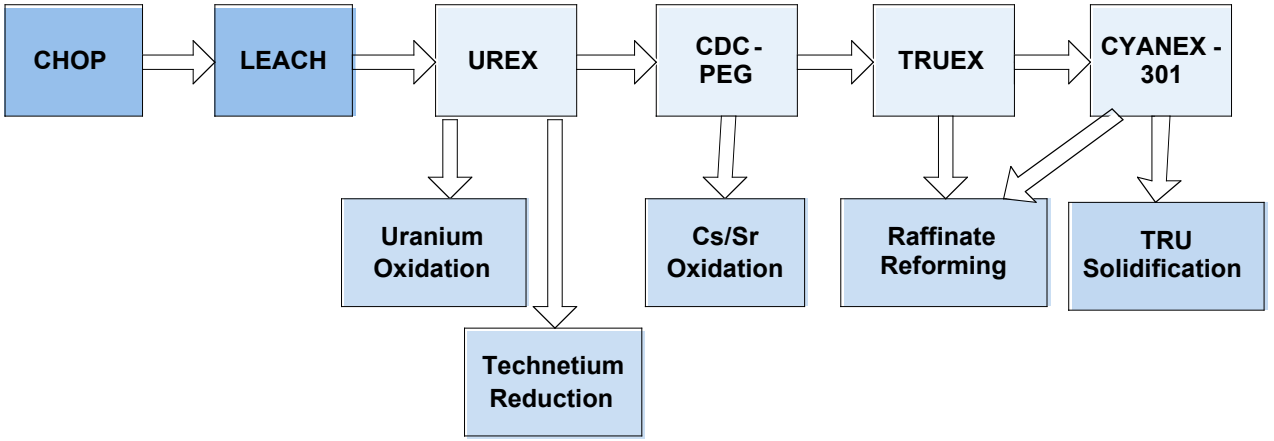
- Use process-specific data collected for a variety of aqueous nuclear fuel processing technologies to predict chemical behavior

**Expanded Scope**

- Generate a benchmark model for an aqueous processing facility
- Improve both the accuracy and precision of models, targeting plant design and construction optimization
- Integrate plant design into systems analysis studies
  - Determine regulatory, economic, physical, and environmental impacts

# *Example of key processes in an aqueous reprocessing plant*

- Actual processes will vary with fuel and product targets
- Extensive heat and energy integration, and materials recycle are required to optimize operations and minimize waste

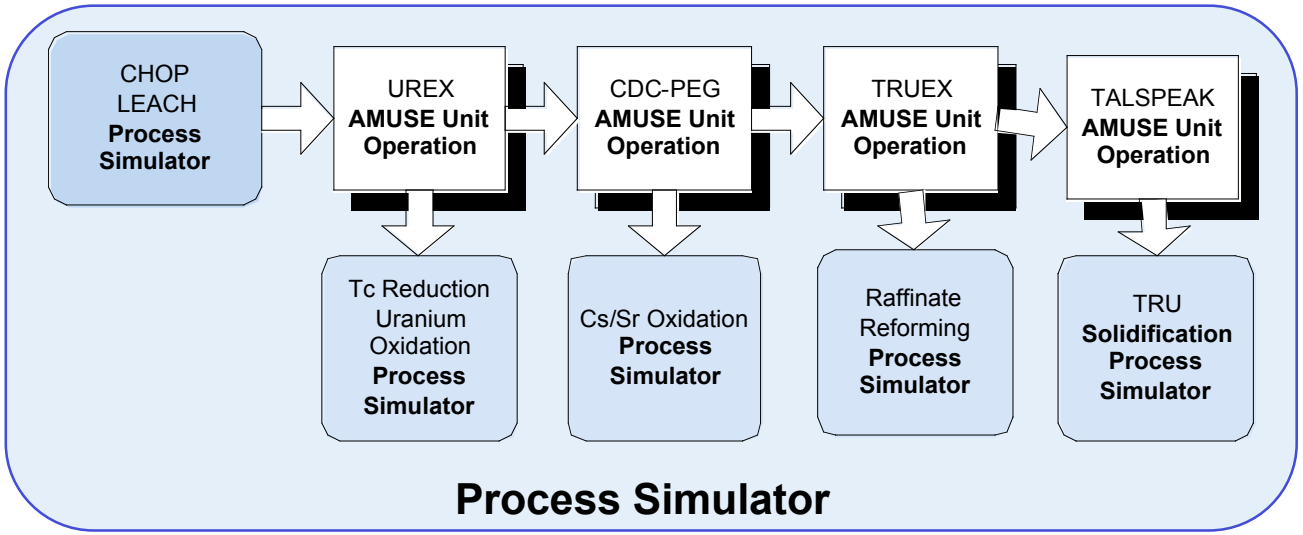


# *The Argonne Model for Universal Solvent Extraction (AMUSE)*

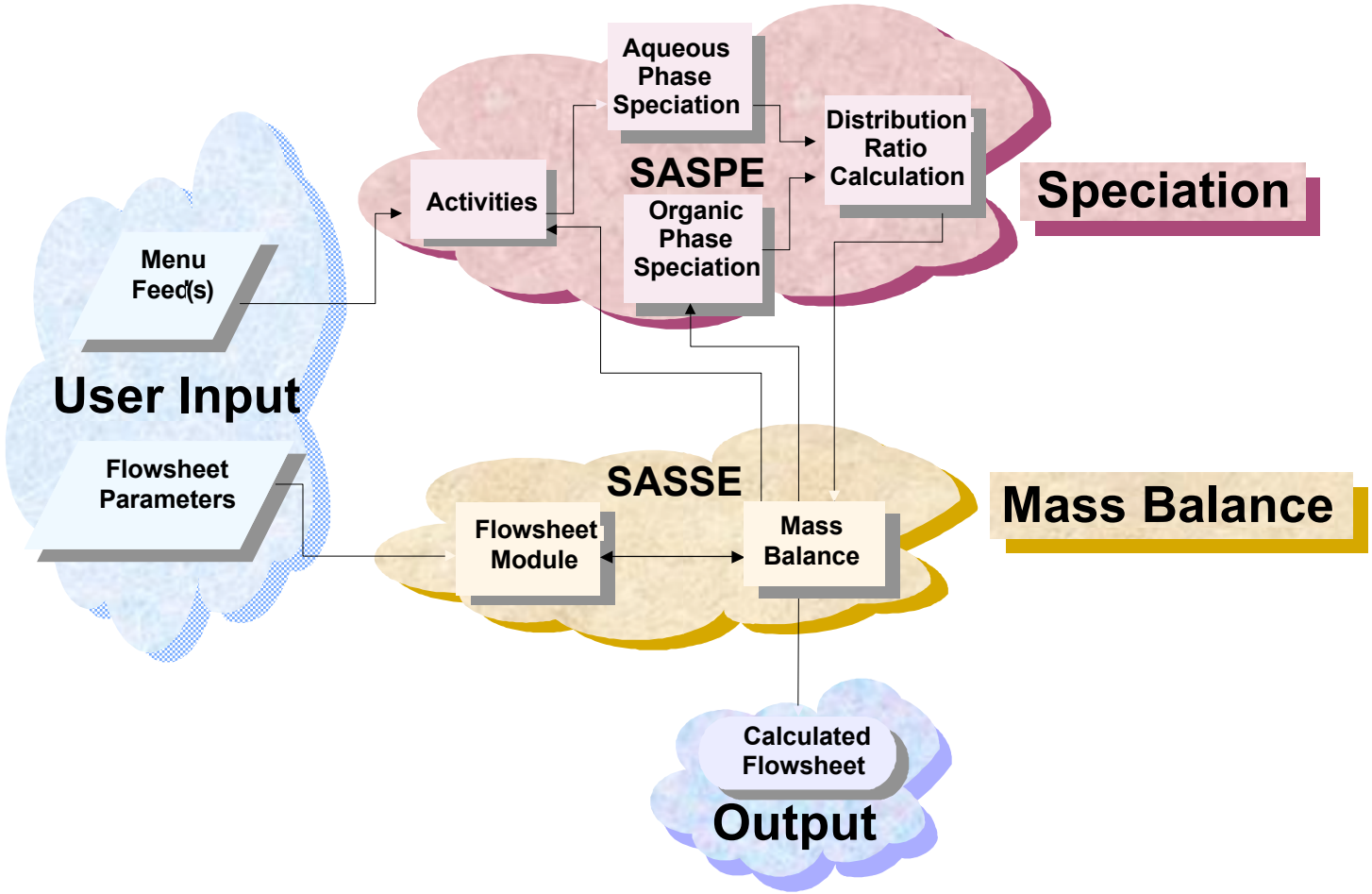
- User input:
  - Type of solvent
  - Composition of feeds
  - Solvent extraction equipment
- Calculates a steady-state solvent extraction flowsheet:
  - Flow rates
  - Number of stages
  - Concentrations of all components present in all effluent streams
  - Temperature
- Displays compositions of all streams in the form of Excel charts and tables

# *AMUSE integration with process simulator*

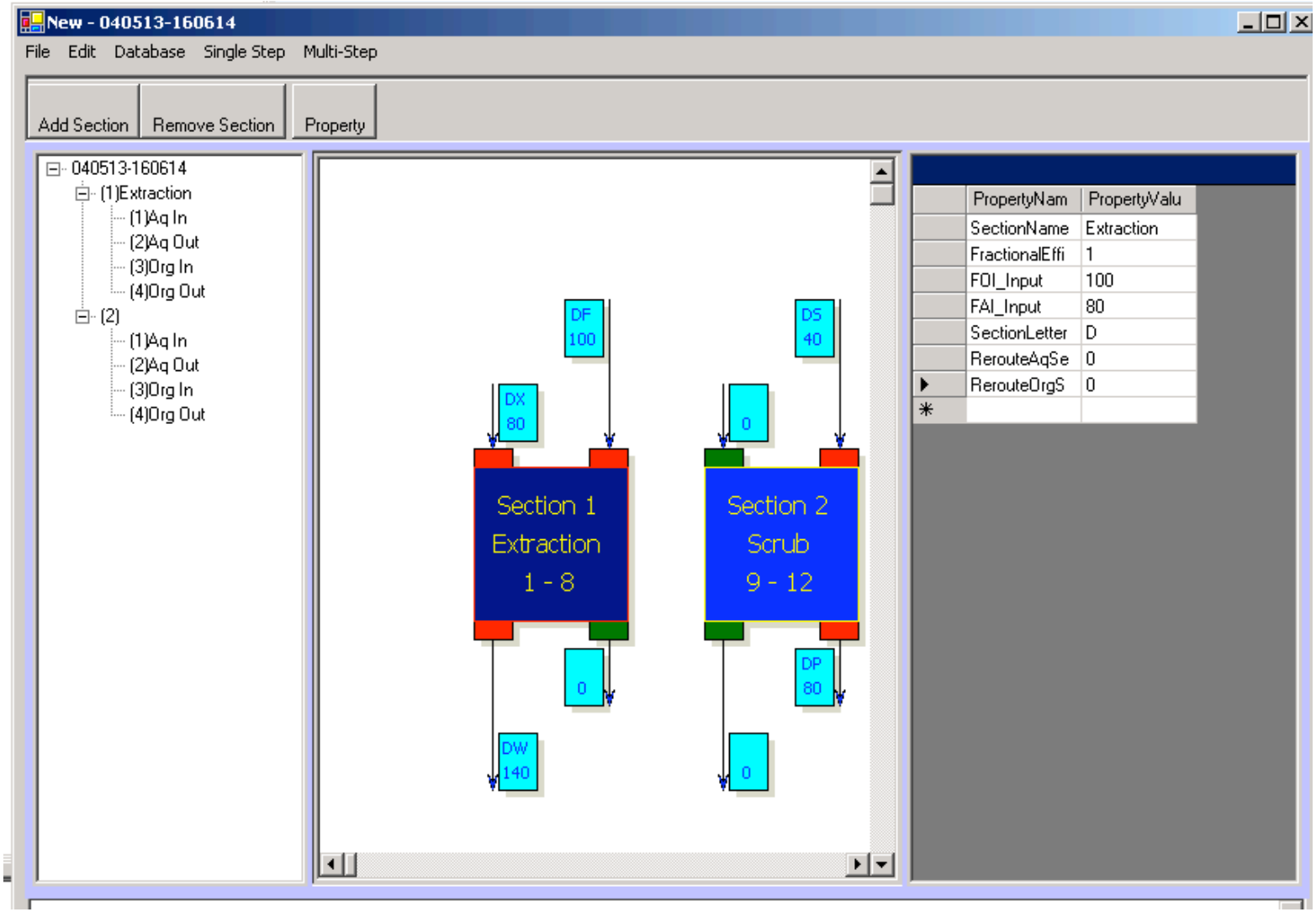
- To simulate a spent fuel treatment facility, AMUSE treats each solvent extraction process as one unit operation
- Unit operations will be integrated with the process simulation package
  - The process simulation package must communicate with AMUSE



# Structure of AMUSE Code



# AMUSE Graphical User Interface



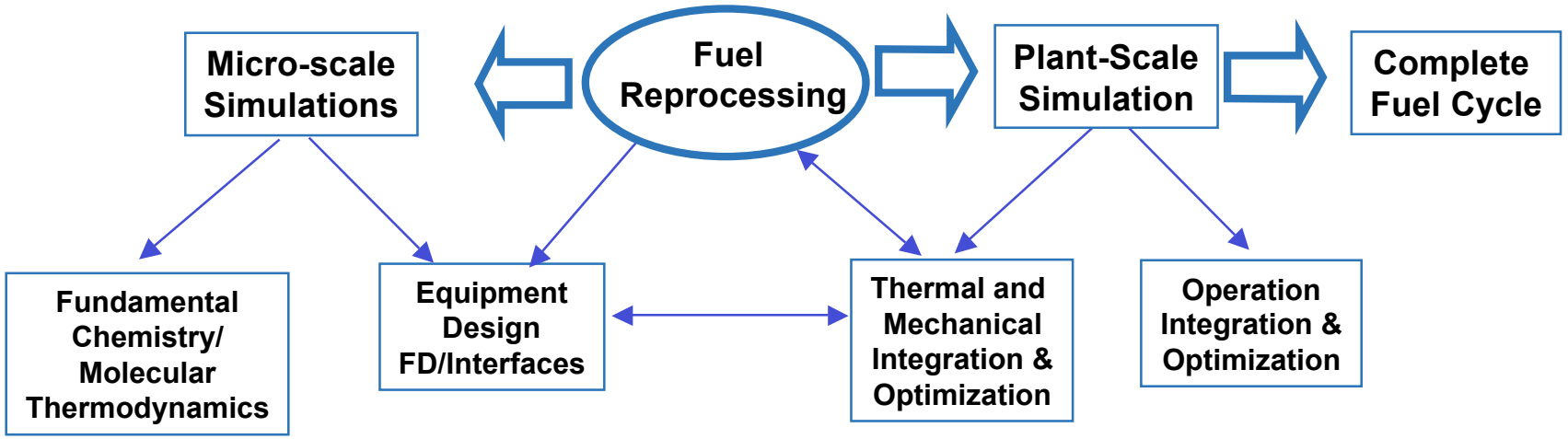
# *Solvent extraction process design and modeling with AMUSE*

- Developed using chemically relevant equilibria for actinides, fission products, and matrix constituents of nuclear fuels
- Design and optimize solvent extraction flowsheets
  - PUREX, UREX, TRUEX, NPEX, SREX and CSSX
  - Adding CCD-PEG and TALSPEAK
- Perform sensitivity analysis to determine key process variables and their control bound
  - Flow rates, number of stages, concentration of feed components, concentration of solvent, temperature
- Output includes speciation, partitioning, and mass balance information that can be used to estimate chemical processing yields
- Used in nuclear processing facilities across the DOE complex

# *Integration of AMUSE with process and systems analysis*

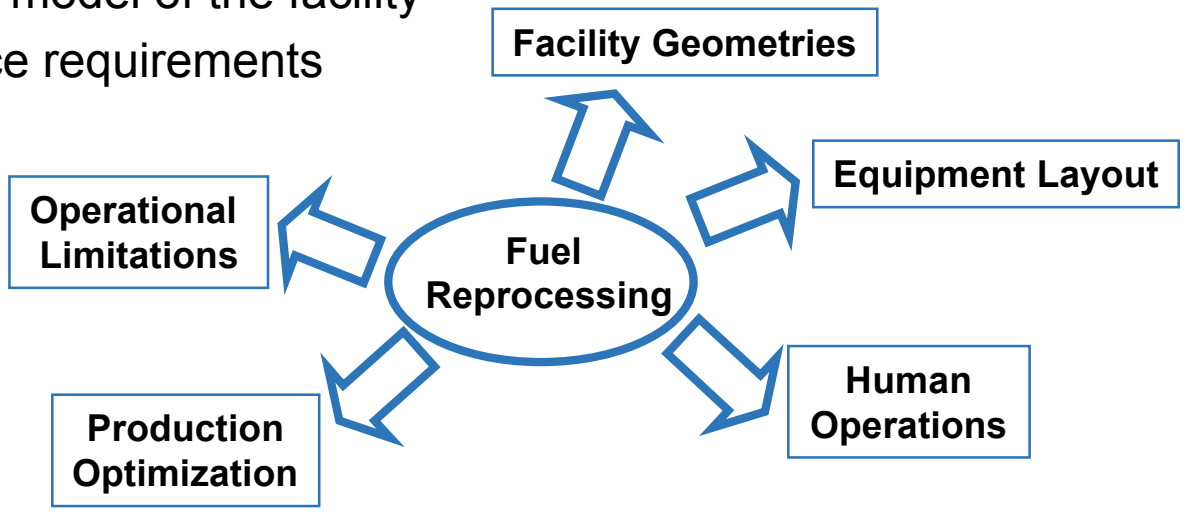
- AMUSE can be used to integrate specific solvent extraction processes into facility design and optimization software
  - Use information to size equipment and optimize layout
  - Plant scaling information can be refined using detailed chemical process simulation routines (e.g., ASPEN or in-house software)
  - Dynamic system simulators (e.g., Extend) can be used to generate preliminary cost estimates of plant construction and operation

# *Extending simulation of fuel reprocessing*

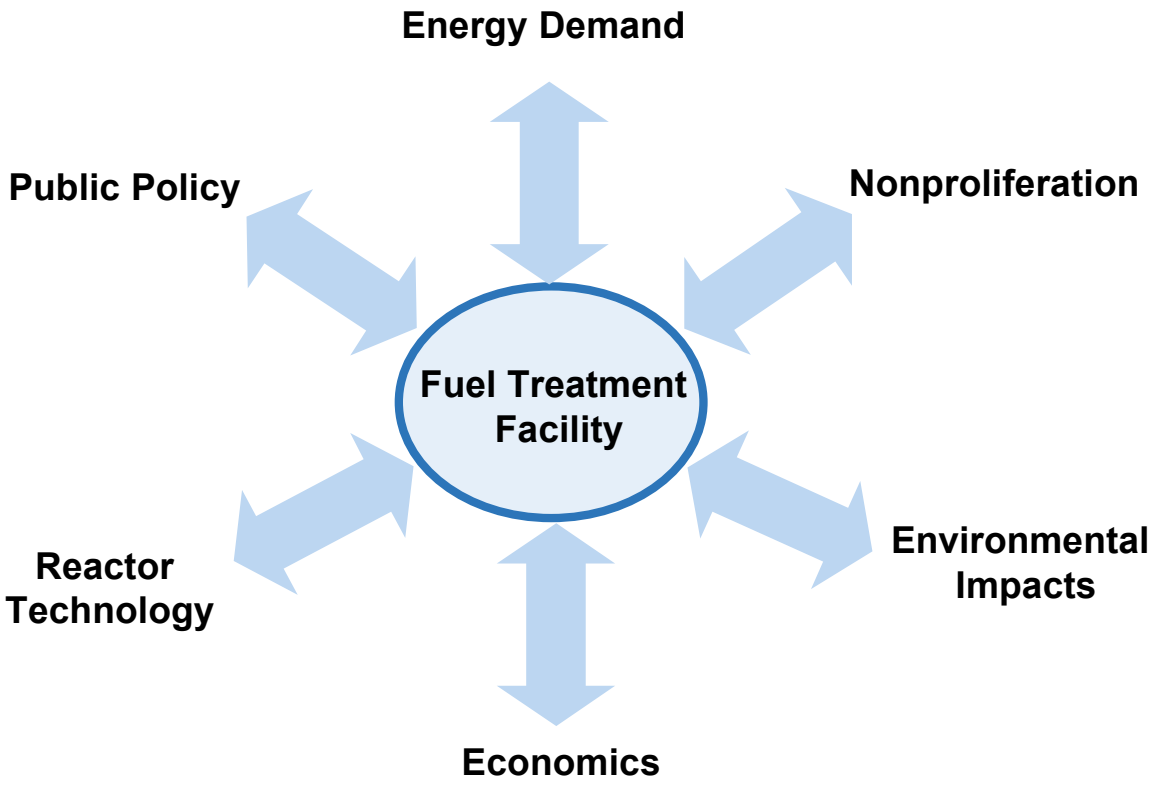


# *Integration of total process simulation with facility layout simulator*

- Optimize facility using operations model
  - Evaluate equipment layout to minimize materials transfer, to simplify access to services, and to optimize equipment spacing
  - Verify facility design for throughput requirements
  - Identify design shortcomings
  - Provide efficiency data on resources
  - Determine operational bottlenecks
  - Test proposed changes for effectiveness
- Develop an operations model of the facility
- Specify control interface requirements



# *Integration of fuel treatment facility with systems analysis*



## *FY06 AFCI AMUSE Milestones*

- Summarize all unit operations needed for an aqueous reprocessing facility using UREX+3 as the reference process
- Define programming requirements for incorporation of AMUSE into a chemical process simulator code
- Determine which unit operations require additional experimental data
- Select case studies to generate a yield database predictor for virtual plant incorporation
  - Next step will incorporate the AMUSE code

# Acknowledgements

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